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PARAMETER ESTIMATION IN MOVING BOUNDARY PROBLEMS

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May 1988

Abstract. We describe an approximation scheme which can be used to estimate unknown parameters in moving boundary problems. The model equations we consider are fairly general nonlinear diffusion/reaction equations of one spatial variable. Here we give conditions on the parameter sets and model equations under which we can prove that the estimates obtained using the approximations will converge to best-fit parameters for the original model equations. We conclude with a numerical example.

Moving boundary problems appear in a large variety of applications. For example, in [4], a nonlinear diffusion equation with moving boundary is derived to model the effects of biofilm growth on the adsorption properties of carbon particles (activated carbon filters are widely used to remove pollutants from water). In [7], parabolic partial differential equations involving moving boundaries are employed to model the elongation of the acrosomal process (a key step in the fertilization of an egg). Finally, the one dimensional, one phase Stefan problem is well known as a model for the melting of ice (see, e.g., [5]).

There are many approaches to solving these problems, both analytical and numerical (see, e.g., [5], [1]). We are interested in numerical methods for the parameter estimation, or inverse problem; we collect data by observing a process which we assume can be modeled by a moving boundary problem. We then try to estimate unknown parameters appearing in the model equations by minimizing a least-squares fit-to-data criterion.

Our approach to solving the parameter estimation problem is that of [3] (see also [2] and the references of both). The infinite dimensional model equations are replaced by an approximating system of ordinary differential equations which have attractive computational features. We estimate the unknown parameters within these approximating equations. We prove that the estimates obtained using the approximate model equations converge in an appropriate sense to best-fit parameters for the original equations.

Specifically, suppose the process in question can be modeled by a moving boundary problem having the following form:

$$
\begin{aligned}
&u_t = \Big(\mathcal{D}(t,x)\, u_x + \mathcal{V}(t,x) u\Big)_x + \rho(u) + f(t,x) \qquad 0 < x < s(t),\ 0 < t \le T;\\
&u(0,x) = u_0(x) \qquad 0 \le x \le s_0;\\
(1)\qquad &\alpha_{11}\Big(\mathcal{D}\, u_x + \mathcal{V} u\Big)\Big|_{x=0} - \alpha_{12}\, u(t,0) = g(t),\\
&\alpha_{21}\Big(\mathcal{D}\, u_x + \mathcal{V} u\Big)\Big|_{x=s(t)} + \alpha_{22}\, u(t,s(t)) = h(t) \qquad 0 < t \le T;\\
&\frac{ds}{dt} = \mathcal{F}(s,u;\gamma) \qquad 0 < t \le T; \qquad s(0) = s_0
\end{aligned}
$$

where one of α_{11} or α_{12}, and one of α_{21} or α_{22} may be zero, and the others are positive; the functional $\mathcal{F}$ may have a variety of forms, to be discussed in more detail below, and γ represents a parameter which is, in general, a function of (t,x). We assume u_0, f, g and h are known; the unknowns in the above system might be any of $\mathcal{D}, \mathcal{V}, \rho, \alpha_{ij}, \gamma$, or s_0, denoted in the following by the vector q. Let us assume here that the observations are in the form of point evaluations, i.e., we have data $\{\hat{u}_{i,j}\}$ corresponding to $u(t_i, x_j)$, where (u,s) is a solution of (1). Then we can formulate

the parameter estimation problem as:

($\mathcal{P}$) Minimize $J(q) = \sum_{j=1}^{m} \sum_{i=1}^{n} \left|\hat{u}_{i,j} - u(t_i, x_j; q)\right|^2$ for $q \in Q$ subject to (u,s) a solution of (1).

Given the general model discussed above, we require further that the following hypotheses be satisfied in order to prove convergence of the parameter estimates.

(H1) We assume that (1) has a unique solution $(u,s) \in C\Big([0,T]; H^1(0,s(t))\Big) \times H^1[0,T]$ with $u(t,x) \geq 0$ and $s(t) \geq \underline{s} > 0$.

(H2) We assume, for any γ, $\mathcal{F}$ satisfies $|\mathcal{F}(s,u_1) - \mathcal{F}(s,u_2)| \leq \lambda(s)|u_1 - u_2|_\infty$ and $|\mathcal{F}(s_1,u) - \mathcal{F}(s_2,u)| \leq \mu(|u|_\infty)|s_1 - s_2|$ with λ and μ both continuous.

(H3) We shall search for the parameters $\mathcal{D}$, $\mathcal{V}$, and γ within compact subsets of $C([0,T] \times [0,s(t)])$, with the additional requirement that there exists a positive constant d such that all $\mathcal{D}$ satisfy $\mathcal{D}(t,x) \geq d$; we search for ρ within a compact subset of $C(0,\bar{u})$ ($\bar{u}$ is an a priori upper bound on u) with the additional requirement that there is a constant L such that all ρ satisfy $|\rho(\theta_1) - \rho(\theta_2)| \leq L|\theta_1 - \theta_2|$ for $\theta_i \in \mathbf{R}$; all α_{ij} and s_0 belong to compact subsets of $\mathbf{R}^+$.

The second hypothesis is satisfied, for example, by the model equations for the activated carbon problem of [4], in which $\mathcal{F}$ involves an integral over the spatial variable of a nonlinear function of u (see the numerical example below). This hypothesis is also satisfied by one of the models of [7] for elongation of the acrosomal process, in which $\mathcal{F}$ involves $u(t,s(t))$. It is not satisfied, however by the Stefan problem, in which $\mathcal{F}$ involves $u_x(t,s(t))$.

In order to derive our approximating equations and to facilitate convergence arguments, we transform the original problem to one of fixed extent, and then, as in [3], we rewrite the equation in variational form. The transformation is accomplished by setting $y = x/s(t)$, letting $U(t,y) = u(t,x)$, $U_0(y) = u_0(x)$, $F(t,y) = f(t,x)$, $D(t,y) = \mathcal{D}(t,x)$, $V(t,y) = \mathcal{V}(t,x)$, and $\Gamma(t,y) = \gamma(t,x)$. Let us assume for definiteness that all boundary parameters are nonzero, and $\alpha_{11} = \alpha_{21} = 1$. We define $X = H^1(0,1)$ and let $\langle \cdot , \cdot \rangle$ denote the inner product in $H^0(0,1)$. We then replace equations (1) by:

$$\langle U_t, \psi\rangle = -\frac{1}{s^2}\langle D\,U_y, \psi_y\rangle - \frac{1}{s}\langle V\,U, \psi_y\rangle + \frac{\dot{s}}{s}\langle y\,U_y, \psi\rangle + \langle \rho(U), \psi\rangle + \langle F, \psi\rangle$$
$$- \frac{1}{s}\left(g(t) + \alpha_{12}U(t,0)\right)\psi(0) + \frac{1}{s}\left(h(t) - \alpha_{22}U(t,1)\right)\psi(1)$$

(2) for all $\psi \in X$, $t \in [0,T]$

$$U(0,y) = U_0(y)$$
$$\dot{s} = \mathcal{F}(s, U; \Gamma) \qquad 0 < t \leq T; \quad s(0) = s_0.$$

We define an approximating subspace $X^N \subset X$ as the span of the set of cubic B-splines defined on a uniform mesh of [0,1] (see [8]), and let $P^N \colon X \to X^N$ be the orthogonal projection in the H^0 topology. Our approximations will then be the solution (U^N, s^N) to the coupled system:

$$\langle U^N_t, \psi\rangle = -\frac{1}{(s^N)^2}\langle D\,U^N_y, \psi_y\rangle - \frac{1}{s^N}\langle V\,U^N, \psi_y\rangle + \frac{\dot{s}^N}{s^N}\langle y\,U^N_y, \psi\rangle + \langle \rho(U^N), \psi\rangle + \langle F, \psi\rangle$$
$$- \frac{1}{s^N}\left(g(t) + \alpha_{12}U^N(t,0)\right)\psi(0) + \frac{1}{s^N}\left(h(t) - \alpha_{22}U^N(t,1)\right)\psi(1)$$

(2^N) for all $\psi \in X^N$, $t \in [0,T]$

$$U^N(0,y) = P^N U_0$$
$$\dot{s}^N = \mathcal{F}(s^N, U^N; \Gamma) \qquad 0 < t \leq T; \quad s^N(0) = s_0.$$

Any unknown variable coefficients must be approximated in addition to the state approximation described above. Just as is described in [2], [3], we approximate variable parameters with linear splines, replacing the parameter set $\mathcal{Q}$ by an appropriate finite dimensional approximating set $\mathcal{Q}^M$. The corresponding computationally tractable parameter estimation problem is given by

$(\mathcal{P}^{N,M})$ Minimize $J^N(q) = \sum_{j=1}^{m}\sum_{i=1}^{n}\left|\hat{u}_{i,j} - U^N\left(t_i, \frac{x_j}{s^N(t_i)}; q\right)\right|^2$ for $q \in \mathcal{Q}^M$ subject to (U^N, s^N) a solution of (2^N).

The system of equations (2^N) represents a system of ordinary differential equations which can be implemented very efficiently on the computer (the details of the numerical aspects will appear in a forthcoming manuscript; a limited discussion has appeared in [6]). The optimization problems $(\mathcal{P}^{N,M})$ are solved for various values of N and M, resulting in a sequence of best-fit estimates. As in [2], [3] the crucial result in proving that solutions of $(\mathcal{P}^{N,M})$ converge (subsequentially) to a solution of $(\mathcal{P})$ is that $\left(U^N(q^{N,M}), s^N(q^{N,M})\right)$ converges (in an appropriate sense) to $\left(U(q), s(q)\right)$ for any sequence $q^{N,M}$ which converges to q (in an appropriate sense). Such a convergence statement can be proven under the hypotheses (H1) - (H3) above, with the addition of:

(H4) There exist constants $\underline{s}$, K such that $s^N(t) \geq \underline{s} > 0$ and $|\dot{s}^N(t)| \leq K$ for all N and $t \in [0,T]$.

The above hypothesis can be met for the same two problems mentioned after (H2). Given a priori knowledge about solutions of (1), one can modify the equation for $\dot{s}^N$ by replacing U^N with a constrained version, $\tilde{U}^N$; this constrained approximate state is constructed in such a way that both (H4) is satisfied, and $|U - \tilde{U}^N|_\infty \leq |U - U^N|_\infty$ (thereby ensuring that $\mathcal{F}(s^N,\tilde{U}^N)$ is a good approximation to $\mathcal{F}(s^N,U^N)$). The details of these arguments will appear elsewhere.

We present the results of a test problem, motivated by the activated carbon model of [4]. Our equations are (1) with

$$\mathcal{F} \equiv \int_0^{s(t)} \left(\frac{u}{u+1} - \gamma(t)\right)dx,$$

$V \equiv 0$, $\rho \equiv 0$, $\alpha_{11} = 1$, $\alpha_{12} = 0$, $\alpha_{21} = 1$, and $\alpha_{22} = 1$. We give the results of two estimations, both of an unknown diffusion coefficient. In both cases, our data is taken to be $u(t_i,0)$ for ten values of time. To generate data, we have first chosen functions u and s, and a "true" diffusion coefficient $\mathcal{D}$, and then determined f, g, h, γ, u_0, and s_0 so that (1) holds. We assume all parameters are known except $\mathcal{D}$. In the first case, we estimate $\mathcal{D} = \mathcal{D}(x)$. The true (transformed) coefficient is given by $D(y) = e^{-y}$. In Figure 1, we have plotted the result of the estimation, using M=5 for the parameter estimation and N=6 for the state approximation. For the second example, we estimate $\mathcal{D} = \mathcal{D}(t)$, with the true coefficient given by $\mathcal{D} = D(t) = \cos(t)$. The results of this estimation, again using M=5 and N=6, can be seen in Figure 2.

We also refer the interested reader to [7], where an example of the Stefan problem appears. As mentioned above, the Stefan problem violates (H2), however, the numerical method is nonetheless successful.

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References

[1] J. Albrecht, L. Collatz, and K.-H. Hoffman (eds.), Numerical Treatment of Free Boundary Value Problems, Birkhauser Verlag, Boston, 1982.

[2] H.T. Banks and P. Daniel Lamm, Estimation of variable coefficients in parabolic distributed systems, IEEE Trans. Auto. Control, 30 (1985), 386-398.

[3] H.T. Banks and K.A. Murphy, Estimation of nonlinearities in parabolic models for growth, predation and dispersal of populations, J. Math. Anal. Appl., to appear.

[4] H.T. Chang and B.E. Rittmann, Mathematical modeling of biofilm on activated carbon, Environ. Sci. Technol., 21 (1987), 273-280.

[5] C.M. Elliott and J.R. Ockendon, Weak and Variational Methods for Moving Boundary Problems (Research Notes in Mathematics, 59), Pitman, London, 1982.

[6] K.A. Murphy, Time-dependent approximation schemes for some problems of parameter estimation in distributed systems, in Proc. 26th IEEE Conf. on Decision and Control, Los Angeles, Dec. 9-11, 1987, 165-169.

[7] A.S. Perelson and E.A. Coutsias, A moving boundary model of acrosomal elongation, J. Math. Biology, 23 (1986), 361-379.

[8] P.M. Prenter, Splines and Variational Methods, Wiley-Interscience, N.Y., 1975.

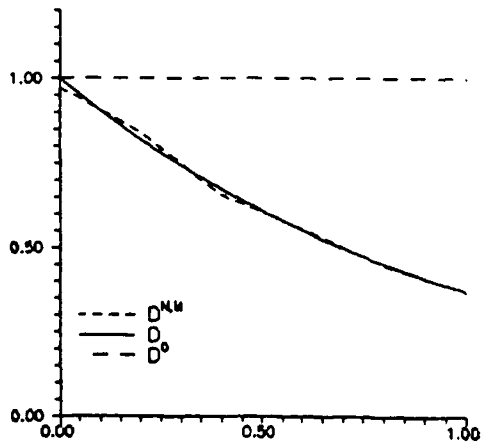

FIGURE 1. Estimation of D(y), M=5

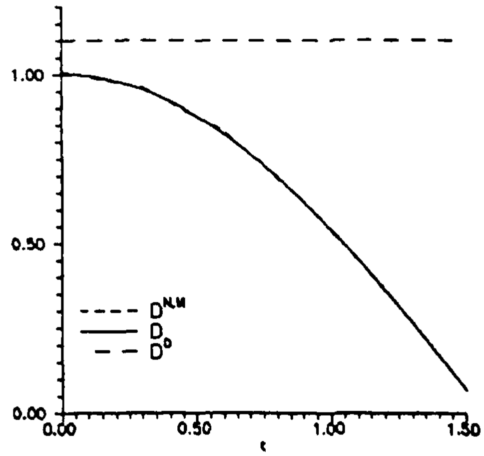

FIGURE 2. Estimation of D(t), M=5